

Reply to Comment on Atomic origin of magneto-crystalline anisotropy in Nd₂Fe₁₄B

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Based on a mean-field analysis of Er₂Fe₁₄B, Kuz'min tries to disprove our statement that $B_{20}^{(f)}$ is opposite in sign to $B_{20}^{(g)}$ in Nd₂Fe₁₄B. Unfortunately, Ref. 1 never makes this statement and it is entirely due to Kuz'min. We used negative values for both parameters and we are pleased that Kuz'min's evaluation supports this choice. The different behavior of the f and g sites is a result of the fourth-order crystal field parameters. In addition, for spins that are not collinear, one also needs to consider the $B_{2,-2}$ crystal-field parameters. Both effects are neglected by Kuz'min, who takes as a starting point that crystal-field effects are small and that the spins of the different Nd sites are always collinear, which is inconsistent with our experimental observations. It is correct that fourth-order terms decay more rapidly, but the measurements are done close to $T \cong \frac{1}{2}T_c$, where the Nd moments are reduced by only $\sim 30\%$ with respect to their saturated moment for $T \rightarrow 0$ K [2]. In addition, Kuz'min's estimate for the temperature dependence of the anisotropy effects is based on a thermal averaging with a Boltzmann distribution containing only the magnetic part of the Hamiltonian. This approach forces the crystal-field effects to disappear at the critical temperature, excludes the presence of magnetic anisotropy in paramagnetic systems at any temperature, and clearly underestimates the anisotropy effects. Although the fourth-order crystal-field parameters have become weaker relative to the second-order terms, the change is insufficient to affect the conclusions of our paper.

Kuz'min concludes that the magnetization of Fe and Nd sublattices cannot deviate from collinearity by more than 2 degrees. This relies on having the same exchange fields at $4f$ and $4g$ Nd sites, and for them to overwhelm crystal field effects at room temperature. However, R-Fe exchange fields [3] are known to differ significantly for the inequivalent $4f$ and $4g$ sites, by $\approx 20\%$ for R=Nd and $\approx 50\%$ for R=Er (resulting in $\alpha = 0.4$ instead of 0.01 and invalidating Eq. 1 of this *Comment*). In addition, exchange and crystal fields acting on R ions in R₂Fe₁₄B are of the same order of magnitude [4–7], the R-Fe exchange coupling not strong enough to ensure a rigid rotation of R and Fe magnetizations [5, 6].

Mean-field approaches such as Kuz'min's cannot explain recent element- and site-specific results showing that Nd and Fe sublattices deviate from collinearity by 30 degrees or more below the ~ 135 K spin reorientation

transition (SRT). Significant deviations from collinearity are also detected between Nd moments at inequivalent crystal sites [2, 8] (see Fig. 1). Mean-field approaches [4, 9] lead to the incorrect conclusion that Nd and Fe sublattices maintain collinearity within a few degrees. This clearly indicates that element- and site-specific information is a must in gaining a fundamental understanding of the competing interactions in R₂Fe₁₄B compounds.

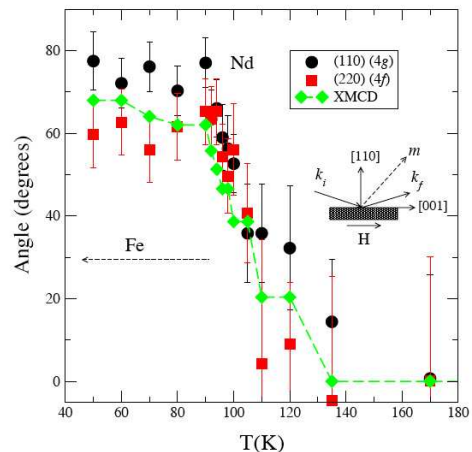


FIG. 1. (color online) Orientation of site-specific Nd moments through the SRT of Nd₂Fe₁₄B. The moments deviate from the c -axis towards the $[110]$ direction. The Fe sublattice reorients by $\sim 30^\circ$ [8]. X-ray magnetic circular dichroism (XMCD) averages over the inequivalent Nd sites.

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